APPENDIX B
USER MANUAL FOR QUAL2E-UNCAS

I. Introduction

The following sections provide instructions for assembling the two application-specific input data files for an UNCAS simulation. The first provides the general specifications for the uncertainty analysis to be performed, and the second contains the input uncertainty information for each input variable.

II. General Specification File; ****.DAT

This data file, named and prepared by the user, contains the general requirements for performing a QUAL2E-UNCAS simulation. This input data file consists of nine data types, as follows.

UNCAS Data Type	Description
1	Heading
2	System Title
3	Uncertainty Option
4	Input Condition
5	Intermediate Output
6	Output Variables
7	Output Locations
8	Input Variables
9	Ending

Data Types 1 through 7 are read by subroutine UNDATA, whereas Types 8 and 9 are read by subroutines INSENS or IFOAMC as necessary. In all UNCAS data types, the first 30 columns contain default data type descriptive information (see UNCAS Input Coding Form).

A. UNCAS Data Type 1 - Heading.

This data type is a default header line for the beginning of the UNCAS general specification file. It consists of one line and is prepared in the following format.

Entry - Text	Position
"UNCAS1___*HEADING____________*"	Columns 1-30
"QUAL2E UNCERTAINTY ANALYSIS"	Columns 31-57

Note: The underscore, "_" indicates a space.

B. UNCAS Data Type 2 - System Title.

This data type contains a user-supplied descriptive title (50 alpha-numeric characters) for the uncertainty simulations. It consists of one line and is formatted as follows.

Entry	Position
"UNCAS2___*SYSTEM_TITLE_______*"	Columns 1-30
User Title	Columns 31-80

C. UNCAS Data Type 3 - Uncertainty Option

Data type 3 is where the user specifies the particular type of uncertainty analysis to be performed. The descriptive text for this data type appears in the first 30 columns as follows.

"UNCAS3___*UNCERTAINTY_OPTION-*"

There are three uncertainty options--sensitivity analysis, first order error analysis, and monte carlo simulation. Also, if first order or monte carlo are selected, the user must supply the magnitude of the input pertubation, or number of monte carlo simulations, respectively. Data type 3 consists of one line prepared with the descriptive text described above, followed by one of these three options.

Entry	Position
"SENSITIVITY ANALYSIS"	Columns 31-50
or	
"FIRST ORDER ERROR ANALYSIS;"	Columns 31-57
Magnitude of input perturbation, %*	Columns 59-64
" % PERTURBATION"	Columns 66-79
or	
"MONTE CARLO SIMULATION:"	Columns 31-53
Number of monte carlo simulations	Columns 59-64
"SIMULATIONS"	Columns 66-76

(* Enter as a percent. If not specified, a default value of 5% is used.)

Note: UNCAS tests the four alphanumeric characters in columns 31-34 (i.e. "SENS", "FIRS", or "MONT") to determine the uncertainty analysis option desired.

D. UNCAS Data Type 4 - Input Condition.

This data type provides UNCAS with information concerning the particulars of the inputs to be modified. The 30 column descriptive text for this line of data is:

"UNCAS4___*INPUT_CONDITION____*"

If the sensitivity analysis option is being exercised, data type 4 conveys to UNCAS whether the inputs (specified in Data Type 8) are to be perturbed (a) singly or in groups or (b) using a factorial design strategy. For the factorial design option, the user must specify the number of input variables in the design. Currently UNCAS accommodates only 2 or 3 variable factorial designs. For sensitivity analysis, UNCAS data type 4 is completed with one of the following two selections.

Entry	Position
"SINGLE/MULTIPLE PERTURBATIONS"	Columns 31-59
or	
"2-LEVEL FACTORIAL DESIGN"	Columns 31-54
Number of input variables (2 or 3)	Column 63
"VARIABLES"	Columns 64-73

If the first order error analysis or the monte carlo simulation option is selected, data type 4 is used to specify which of the generic groups of input variables are to be varied. These groupings are defined according to the QUAL2E input data types and are specified using the following alphanumeric code.

QUAL2E Input Variables	QUAL2E Data Types	UNCAS Alphanumeric Code
Global	1, 1A, 1B	GLBL
Hydraulic/Climatology	5, 5A	HYDR
Reaction Coefficient	6, 6A, 6B	RXNC
Incremental Flow	8, 8A	FFIF
Headwater Conditions	10, 10A	FFHW
Point Loads	11, 11A	FFPL
Dams	12	FFDM

For the first order and monte carlo options, data type 4 is completed with one of the following two selections.

Entry	Position
"ALL INPUTS"	Columns 31-40
or	
"GENERIC GROUPS"	Columns 31-44
1st alphanumeric code	Columns 47-50
2nd alphanumeric code	Columns 52-55
3rd alphanumeric code	Columns 57-60
4th alphanumeric code	Columns 62-65
5th alphanumeric code	Columns 67-70
6th alphanumeric code	Columns 72-75
7th alphanumeric code	Columns 77-80

Any number (from 1-7) of groups may be specified and only the QUAL2E inputs in that (those) group(s) will be perturbed in the uncertainty analysis. Note: UNCAS tests the four alphanumeric characters in columns 31-34 (i.e. "SING," "2-LE," "ALL_" or "GENE") to determine the input condition desired.

E. UNCAS Data Type 5 - Intermediate Output

With data type 5, the user can specify whether any intermediate output is desired. Intermediate output is defined as line printer output for each uncertainty simulation. The 30 column descriptive text for this line of data is:

"UNCAS5___*INTERMED_OUTPUT____*"

UNCAS recognizes three options for intermediate output: none, a complete QUAL2E final summary, and a limited output summary. The limited intermediate output summary consists of an echo print of the inputs that have been perturbed for the uncertainty simulation, a summary of the steady-state temperature and algae convergence computations, and a tabulation of the base and new values of the ouptut variables at the locations specified (UNCAS Data Type 7). Entries for data type 5 are completed with one of the following 3 selections.

Entry	Position
"NONE"	Columns 31-34
or	
"COMPLETE QUAL2E FINAL SUMMARY"	Columns 31-59
or	
"LIMITED"	Columns 31-37

Note: because of the potential for voluminous output, the second and third options are not available for monte carlo simulation. UNCAS tests the four alphanumeric characters in columns 31-34 (i.e. "NONE", "COMP", or "LIMI") to determine the intermediate output desired.

F. UNCAS Data Type 6 - Output Variables.

Data type 6 is used to constrain the list of output variables for which uncertainty results will be computed. These constraints are applied in a manner analogous to the input variable constraints in data type 4. The user simply specifies the generic groups of output variables for which uncertainty results are desired. The 30 column descriptive text for this line of data is:

"UNCAS5___*OUTPUT_VARIABLES___*"

The generic output groups are named "HYDRAULIC," "QUALITY," AND "INTERNAL." The hydraulic group consists of 10 output variables (flow, depth, velocity, dispersion,etc.) associated with the hydraulic output from QUAL2E. The quality group consists of the values of the 17 state variables simulated by QUAL2E. The internal group is made up of 9 diagnostic or internal variables associated with the algal, nutrient, light interactions in QUAL2E (i.e. algal growth rate p minus r and p/r ratio, light and nutrient factors in the growth rate computation, nitrification inhibition factor, etc.). This data type is completed by adding the names of the generic output variable groups to the data type 6 line as follows.

Entry	Position
Generic Output Group 1	Columns 31-40
Generic Output Group 2	Columns 46-55
Generic Output Group 3	Columns 61-70

Note: UNCAS tests the four alphanumeric characters in columns 31-34, 46-49, and 61-64 (i.e., "HYDR," "QUAL," or "INTE") to determine the generic group of output variables to be analyzed. They may be placed in any order in the appropriate positions.

G. UNCAS Data Type 7 - Output Locations.

This data type is used to define the locations in the basin where the output variables are to be examined for uncertainty analysis. The 30 column descriptive text for UNCAS data type 7 is:

"UNCAS7___*OUTPUT_LOCATIONS___*"

UNCAS will accept a maximum of 5 locations in the basin for output analysis. They are supplied as a single line in the form of reach and element number as follows.

Entry	Position
Location 1 (Reach and Element Number)	Columns 33-35, 36-38
Location 2 (Reach and Element Number)	Columns 41-43, 44-46
Location 3 (Reach and Element Number)	Columns 49-51, 52-54
Location 4 (Reach and Element Number)	Columns 57-59, 60-62
Location 5 (Reach and Element Number)	Columns 65-67, 68-70

Note: Reach and element numbers must be right-justified in their appropriate column fields.

H. UNCAS Data Type 8 - Input Variables

This data type is used to supply UNCAS with the input variable specifications for performing sensitivity analysis. It is not required for the first order error analysis and monte carlo simulation options. The 30-column descriptive text for UNCAS data type 8 is:

"UNCAS8___*INPUT_VARIABLES*"

This data type will consist of one or more lines, depending on how many sensitivity simulations are desired and/or on how many variables are to be sensitized in a given simulation.

The information in this data type is designed to handle any of three different input conditions for sensitivity analysis: one variable at a time, variables in groups, or factorially designed. The data on each line consists of specifying the input condition, the number of variables to be sensitized, the name of the input variable, and the magnitude of the perturbation.

For a one variable at a time simulation, one line of input is required as follows.

Entry	Position
"SINGLE"	Columns 31-36
Number of inputs perturbed	Column 45
Input variable code	Columns 48-56
Magnitude of perturbation, %	Columns 58-63

The number of inputs perturbed with this option is always 1. The input variable codes are 8 alphanumeric characters as shown in Table B-1. This line of data may be repeated for one variable at a time sensitivity simulations with other variables or other levels of perturbation.

For sensitivity analyses where more than one variable is perturbed, one line of input is required for each input variable to be altered, as follows.

Entry	Position
"MULTIPLE"	Columns 31-38
Number of inputs perturbed	Column 45
Input variable code	Columns 49-56
Magnitude of perturbation, %	Columns 58-63

UNCAS limits the number of inputs perturbed for this option to be either 2 or 3, thus requiring 2 or 3 lines of UNCAS data type 8, respectively. The input variable codes are shown in Table B-1. As with one variable at a time simulations, groups of multiple variable sensitivity simulations may appear one after the other in this data type.

For sensitivity analysis using variables in a factorically designed configuration, one line of input is required for each input variable as follows.

Entry	Position
"FACTORIAL"	Columns 31-39
Number of Inputs perturbed	Column 45
Input variable code	Columns 49-56
Magnitude of perturbation, %	Columns 58-63

UNCAS limits the number of inputs perturbed in the factorial design option to be either 2 or 3, thus requiring 2 or 3 lines of UNCAS data type 8, respectively. The input variable codes are shown in Table B-1. UNCAS automatically sets up conditions for each of the 4 or 8 factorial design simulations. As with the other sensitivity analysis options, groups of factorial design conditions may appear one after the other in this data type.

Note: UNCAS tests the four alphanumeric characters in column 31-34 (i.e. "SING", "MULT", and "FACT") to determine the sensitivity analysis option desired. UNCAS also allows the user to mix the sensitivity analysis option types in a single execution of the program; however, the maximum number of sensitivity simulations is 120. This data type is not required for the first order error analysis or monte carlo simulation options.

I. UNCAS Data Type 9 - Ending.

This data type is a default ending line that signifies the end of the general specification file. It consists of one line and is prepared in the following format.

Entry - Text	Position
"UNCAS9___*ENDING_____________*"	Columns 1-30
"ENDUNCERTAINTY"	Columns 31-44

III. Input Variance Data File; INVAR.DAT.

This data file contains the uncertainty information for each input variable in QUA12E. An example of this file containing a set of default data is provided with the UNCAS package. However, the user must adjust the default data to values suitable for the particular case being modeled. The data contained in INVAR.DAT consists of the variable code name, its QUA12E data type, its coefficient of variation, and its probability density function. The first two lines of the file are title and header lines. Subsequent lines contain the variance information, formatted as follows.

Entry	Position
Input Variable Name	Columns 3-30
Input Variable Code	Columns 36-43
QUAL2E Data Type	Columns 49-50
Coefficient of Variation	Columns 56-60
Probability Density Function	Columns 68-69

The input variable codes are shown in Table B-1. The two character codes for probability density function are "NM" for normal distribution and "LN" for log-normal.

TABLE B-1 INPUT VARIABLE NAME CODES

Input variable Name	Input Code	QUAL2E Data Type
Evaporation coef - AE	ECOEF-AE	1
Evaporation coef - BE	ECOEF-BE	1
Oxygen uptake by NH3 oxdtn	NH3OXYUP	1A
Oxygen uptake by NO2 oxdtn	NO2OXYUP	1A
Oxygen prod by algae grwth	AGYOXYPR	1A
Oxygen uptake by algy resp	AGYOXYUP	1A
Nitrogen content of algae	AGYNCON	1A
Phosphorus content of algy	AGYPCON	1A
Algy max spec growth rate	AGYGROMX	1A
Algae respiration rate	AGYRESPR	1A
Nitrogen half sat'n coef	NHALFSAT	1A
Phosphorus half sat'n coef	PHALFSAT	1A
Linear alg self shade coef	AGYEXTLN	1A
Non-lin alg self shade co	AGYEXTNL	1A
Light sat'n coefficient	LSATCOEF	1A
Light averaging factor	LAVGFACT	1A
Number of daylight hours	NUMBDLH	1A
Total daily solar radt'n	TDYSOLAR	1A
Alg pref for ammonia-N	APREFNH3	1A
Alg to temp solar factor	A/TFACT	1A
Nitrification inhib fact	NHIBFACT	1A
5-D to ult BOD conv r-cof	5TOUBODK	1
Temp coef BOD decay	TC/BODDC	1B
Temp coef BOD settling	TC/BODST	1B
Temp coef O2 reaeration	TC/REAER	1B
Temp coef sed O2 demand	TC/SOD	1B
Temp coef organic-N decay	TC/NH2DC	1B
Temp coef organic-N set	TC/NH2ST	1B
Temp coef ammonia decay	TC/NH3DC	1B
Temp coef ammonia srce	TC/NH3SC	1B
Temp coef nitrite decay	TC/NO2DC	1B
Temp coef organic-P decay	TC/PRGDC	1B
Temp coef organic-P set	TC/PRGST	1B
Temp coef diss-P source	TC/PO4SC	1B
Temp coef algy growth	TC/ALGRO	1B
Temp coef algy respr	TC/ALRES	1B
Temp coef algy settling	TC/ALSET	1B
Temp coef coli decay	TC/CLIDC	1B
Temp coef ANC decay	TC/ANCDC	1B
Temp coef ANC settling	TC/ANCST	1B
Temp coef ANC source	TC/ANCSC	1B
Daily averaging option	DIURNOPT	1A
Light function option	LFNOPTN	1A
Algae growth calc option	AGYGROPT	1A

Table B-1 (continued)

Input Variable Name	Input Code	QUAL2E Data Type
Dispersion corr constant	DISPSN-K	5
Coef on flow for velocity	COEFQV-A	5
Expo on flow for velocity	EXPOQV-B	5
Coef on flow for depth	COEFQH-C	5
Expo on flow for depth	EXPOQH-D	5
Manning's roughness n	MANNINGS	5
Side slope 1	TRAP-SS1	5
Side slope 2	TRAP-SS2	5
Bottom width	TRAP-WTH	5
Slope of channel	TRAP-SLP	5
Mean elevation of reach	ELEVATIN	5A
Dust attenuation coef	DUSTATTN	5A
Fraction of cloudiness	CLOUD	5A
Dry bulb air temperature	DRYBULB	5A
Wet bulb air temperature	WETBULB	5A
Barometric pressure	ATMPRES	5A
Wind speed	WINDVEL	5A
CBOD oxidation rate	BOD DECA	6
CBOD settling rate	BOD SETT	6
SOD uptake rate	SOD RATE	6
Reaeration rate option 1	K2-OPT1	6
Coef on flow for K2 opt-7	CQK2-OP7	6
Expo on flow for K2 opt-7	EQK2-OP7	6
Coef for K2 (TSIV) opt-8	K2COEF-8	6
Slope for K2(TSIV) opt-8	K2SLOP-8	6
Organic-N hydrolysis rate	NH2 DECA	6A
Organic-N settling rate	NH2 SETT	6A
Ammonia-N decay rate	NH3 DECA	6A
Ammonia-N bethal source	NH3 SRCE	6A
Nitrite-N decay rate	NO2 DECA	6A
Organic-P hydrolysis rate	PORG DEC	6A
Organic-P settling rate	PORG SET	6A
Dissolved-P Benthal srce	DISP SRC	6A
Chla to algae ratio	CHLA/ART	6B
Algae settling rate	ALG SETT	6B
Light ext coefficient	LTEXTNCO	6B
Coliform decay rate	COLI DEC	6B
ANC decay rate	ANC DECA	6B
ANC settling rate	ANC SETT	6B
Initial temperature	INITTEMP	7A
Reaeration equation opt.	K2OPTION	6
Incremental flow	INCRFLOW	8
Incr-temperature	INCRTEMP	8
Incr-dissolved oxygen	INCRDO	8

Table B-1 (continued)

Input Variable Name	Input Code	QUAL2E Data Type
Incr-BOD	INCRBOD	8
Incr-consv min 1	INCRCM1	8
Incr-consv min 2	INCRCM2	8
Incr-consv min 3	INCRCM3	8
Incr-arbitrary non-cons	INCRANC	8
Incr-coliform	INCRCOLI	8
Incr-algae	INCRCHLA	8A
Incr-organic-N	INCRNH2N	8A
Incr-ammonia-N	INCRNH3N	8A
Incr-nitrite-N	INCRNO2N	8A
Incr-nitrate-N	INCRNO3N	8A
Incr-organic-phos	INCRPORG	8A
Incr-dissolved-phos	INCRDISP	8A
Headwater flow	HWTRFLOW	10
Hwtr-temperature	HWTRTEMP	10
Hwtr-dissolved oxygen	HWTRDO	10
Hwtr-BOD	HWTRBOD	10
Hwtr-consv min 1	HWTRCM1	10
Hwtr-consv min 2	HWTRCM2	10
Hwtr-consv min 3	HWTRCM3	10
Hwtr-arbitrary non-cons	HWTRANC	10A
Hwtr-coliform	HWTRCOLI	10A
Hwtr-algae	HWTRCHLA	10A
Hwtr-organic-N	HWTRNH2N	10A
Hwtr-ammonia-N	HWTRNH3N	10A
Hwtr-nitrite-N	HWTRNO2N	10A
Hwtr-nitrate-N	HWTRNO3N	10A
Hwtr-organic-phos	HWTRPORG	10A
Hwtr-dissolved-phos	HWTRDISP	10A
Ptld-trtmnt factor	PTLDTFCT	11
Point load flow	PTLDFLOW	11
Ptld-temperature	PTLDTEMP	11
Ptld-dissolved oxygen	PTLDDO	11
Ptld-BOD	PTLDBOD	11
Ptld-consv min 1	PTLDCM1	11
Ptld-consv min 2	PTLDCM2	11
Ptld-consv min 3	PTLDCM3	11
Ptld-arbitrary non-cons	PTLDANC	11A
Ptld coliform	PTLDCOLI	11A
Ptld-algae	PTLDCHLA	11A
Ptld-organic-N	PTLDNH2N	11A
Ptld-ammonia-N	PTLDNH3N	11A
Ptld-nitrite-N	PTLDNO2N	11A
Ptld-nitrate-N	PTLDNO3N	11A
Ptld-organic phos	PTLDPORG	11A
Ptld-dissolved-phos	PTLDDISP	11A
Dam coefficient a	DAMSACOF	12
Dam coefficient b	DAMSBCOF	12
Fraction of flow over dam	DAMSFRAC	12

QUAL2E - UNCAS INPUT DATA CODING FORM - GENERAL UNCAS SPECIFICATIONS

UNCAS DATA TYPE	INPUT DATA, SHOWING OPTIONS (or) FOR DATA TYPES 3, 4, 5 AND 8
UNCAS1 *HEADING	*QUAL2E UNCERTAINTY ANALYSIS
UNCAS2 *SYSTEM TITLE	*
UNCAS3 *UNCERTAINTY OPTION	*SENSITIVITY ANALYSIS FIRST ORDER ERROR ANALYSIS: ☐ % PERTURBATION MONTE CARLO SIMULATION: ☐ SIMULATIONS
UNCAS4 *INPUT CONDITION	*SINGLE/MULTIPLE PERTURBATIONS 2-LEVEL FACTORIAL DESIGN ☐-VARIABLES GENERIC GROUPS ☐ ☐ ☐ ☐ ☐ ☐ ☐ ALL INPUTS
UNCAS5 *INTERMED OUTPUT	*NONE COMPLETE QUAL2E FINAL SUMMARY * ☐
UNCAS6 *OUTPUT VARIABLES	* ☐ ☐ ☐
UNCAS7 *OUTPUT	* ☐ ☐ ☐ ☐ ☐
UNCAS8 *INPUT VARIABLES	*SINGLE MULTIPLE FACTORIAL
UNCAS9 *ENDING	*ENDUNCERTAINTY

UNCAS1 : (A4,1X,I1)
UNCAS2 : (A4,1X,I1,24X,12A4,A2)
UNCAS3 : (A4,1X,I1,24X,A4,24X,F6.0)
UNCAS4 : (A4,1X,I1,24X,A4,28X,I1) or (A4,1X,I1,24X,A4,11X,7(1X,A4))
UNCAS5 : (A4,1X,I1,24X,A4)
UNCAS6 : (A4,1X,I1,24X,A4,3(A4,11X))
UNCAS7 : (A4,1X,I1,24X,5(2X,2F3.0))
UNCAS8 : (A4,1X,I1,24X,A4,10X,I1,3X,2A4,IX,F6.0)

Notes:

1. All data types consist of 1 line, except UNCAS8 which may have more than one.
2. Blank lines between data types shown here for clarity. Actual input data file has no blank lines.

APPENDIX C

QUAL2E-UNCAS Example Application

A. Introduction

The material in this appendix provides an example of how the uncertainty methodologies in QUAL2E-UNCAS can be applied to a QUAL2E data set. The sole purpose of this section is to demonstrate the utility of uncertainty analysis rather than to provide a definitive analysis of the river system from which the data were obtained. The example input data files and some of the output data files that were used in this application are provided with the model code distributed by the Center for Water Quality Modeling (CWQM).

B. Withlacoochee River Basin

The data used to demonstrate the capabilities of QUAL2E-UNCAS were obtained from a USEPA survey of the Withlacoochee River during October 1984 (Koenig, 1986). In this study, water quality simulations were examined for portions of the river subjected to both municipal and industrial waste loads. In addition there is a significant accretion of flow from groundwater inputs. The river has a uniform low slope, but is characterized by alternating shoals and pools (often in excess of 25 feet deep). Average depths during the survey periods were 5.2 to 14.8 feet, widths were 90 to 140 feet, and flows varied from 150 cfs at the headwater to 660 cfs at the end of the system. Water quality is affected by algal activity resulting from municipal waste discharges above the section of stream studied. The addition of industrial waste at RM 24, however, dramatically reduces light penetration to the extent that the algal population diminishes in the downstream direction.

A location map of the basin is shown in Figure C-1 and a plot of observed and modeled dissolved oxygen concentrations is presented in Figure C-2. Ten state variables were simulated in this study, temperature, dissolved oxygen, carbonaceous BOD, four nitrogen forms, (organic, ammonia, nitrite, and nitrate), two phosphorus forms, (organic and dissolved), and algae as chlorophyll *a*. A summary of the calibrated inputs and their variance estimates for the uncertainty analysis is shown in Table C-1. The calibrated values in general were obtained by adjusting field or laboratory measurements of the specific model inputs. The variance estimates were computed from replicate data taken during the survey period and by inference from other published data. (McCutcheon, 1985 and Bowie *et al.*, 1985)

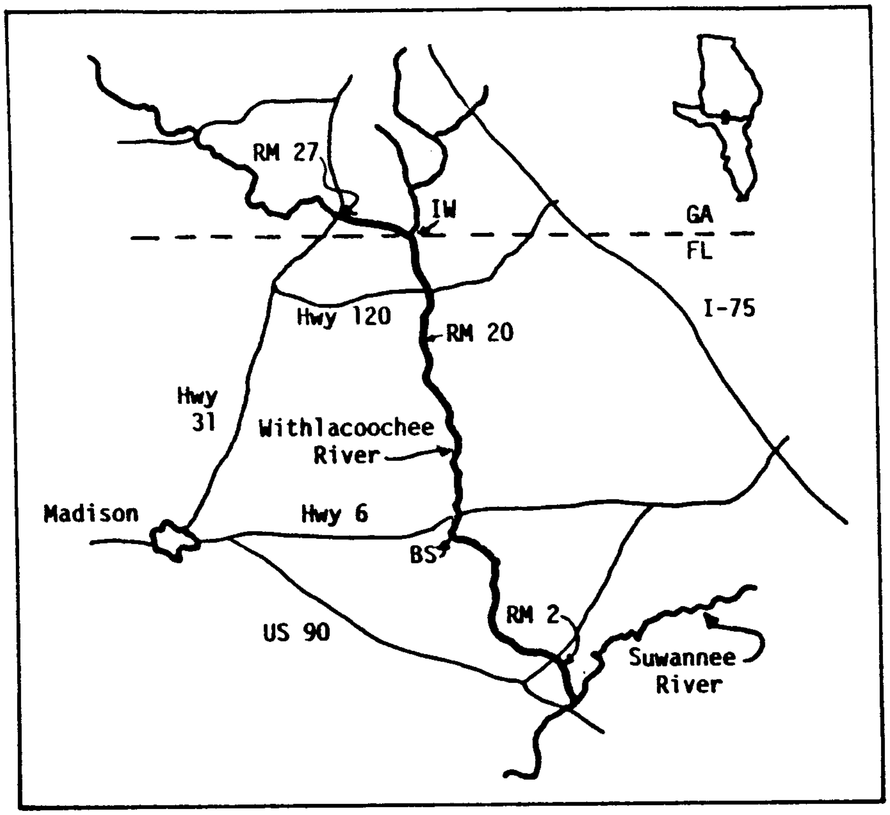

Fig. C-1. Location map of the Withlacoochee River basin.

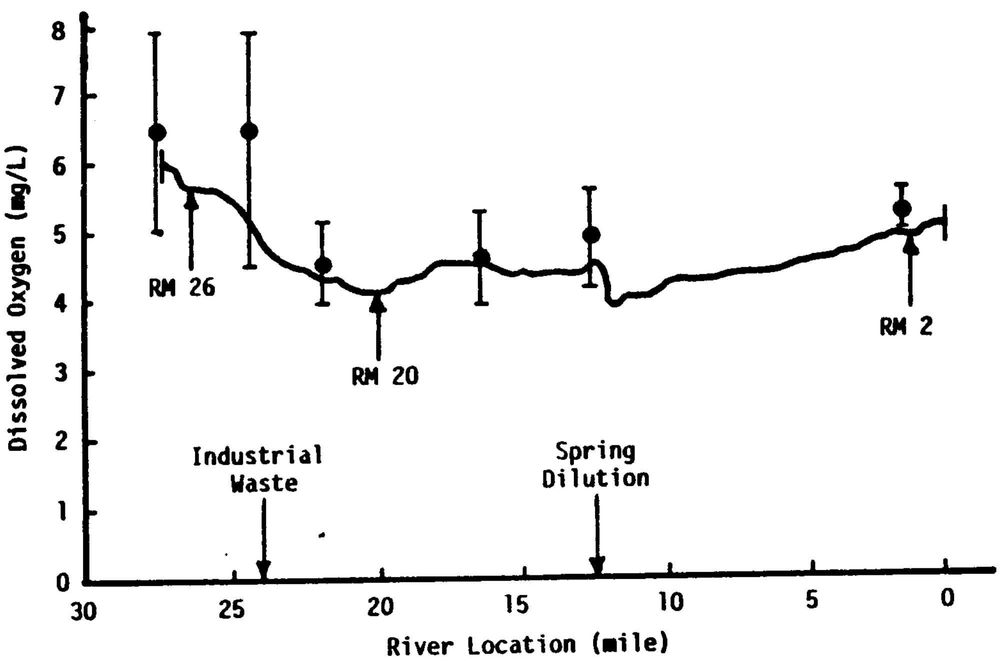

Fig. C-2. Observed and predicted dissolved oxygen concentrations.

C. First Order Error Analysis (FOEA)

Table C-2 shows the first order error analysis (FOEA) results for the output variables of CBOD and DO at three locations in the Withlacoochee system: an upstream location (RM 26), a midpoint near the dissolved oxygen sag (RM 20), and a downstream location (RM 2). For the CBOD sensitivity coefficients in Table C-2a, it is clear that the input forcing functions dominate model sensitivity. In general, point load and headwater flows and CBOD have the largest sensitivity coefficients, however, their effects change with location in the system. Headwater inputs dominate sensitivity in the upper reaches of the river and decrease in importance as one

TABLE C-1 Summary of Input Data for QUAL2E-UNCAS Simulations - Withlacoochee River Survey 1984

Input Parameter or Coefficient	Base Case (Mean) Values	Relative Standard Deviations (%)
Hydraulic Data (7)*		
Flows (cfs)	150 - 660	3%
Depths (ft)	5.2 - 14.8	8%
Velocities (fps)	.12 - .78	8%
Others	a,b	10 - 20%
Reaction Coefficients (8)		
CBOD Decay (1/day)	.04 - .10	15%
Reaeration (1/day)	.08 - .80	13%
SOD (gm/ft^2-day)	.04 - .13	12%
N, P, Algae	a,b	15 - 25%
Algae, Nutrient, Light Coefficients (17)		
Maximum Growth Rate (1/day)	1.3	10%
Respiration Rate (1/day)	.15	10%
Others	a,b	10%
Climatology, Temperature Inputs (23)		
Wet, Dry Bulb Air Temps (^{o}F)	64.3, 74.5	2%
Temperature Coefficients	1.00 - 1.083	3%
Others	a,b	1 - 15%
Headwater, Incremental, Point Loads (27)		
DO, Temperature	a	1 - 3%
CBOD, N, P, Algae	a	8 - 25%

(a) Basin specific values from Koenig, 1986.
(b) Typical values from Table III-3 of this report.

* Value in parentheses is the number input variables of the type indicated.

TABLE C-2 Summary of First Order Simulations for Withlacoochee River

(a) Simulation Variable: CBOD

Input Variable	Relative Std Dev (%)	Sensitivity Coefficients RM 26	RM 20	RM 2	Components of Variance (%) RM 26	RM 20	RM 2
CBOD Decay	15	-.06 (3)*	-.11	-.22	1	2	8
Incr Flow	3	-.05	-.22	-.37 (3)	1	1	1
HW Flow	3	.05	-.44 (3)	-.05	1	1	1
HW Temp	1	-.11 (2)	-.13	-.16	1	1	1
HW CBOD	15	.98 (1)	.24	.18	99	9	6
Ptld Flow	3	.00	.67 (2)	.43 (2)	0	3	1
Ptld CBOD	15	.00	.74 (1)	.69 (1)	0	84	79
Standard Deviation of Simulated CBOD (mg/L)					0.35	0.76	0.27
(%)					15	12	12

(b) Simulation Variable: Dissolved Oxygen

Input Variable	Relative Std Dev (%)	Sensitivity Coefficients RM 26	RM 20	RM 2	Components of Variance (%) RM 26	RM 20	RM 2
Velocity	8	.03	.05	-.26 (2)	1	2	13
CBOD Decay	15	-.02	-.12	-.03	1	9	1
SOD	5	-.05 (3)	-.23	.09	5	20	3
Reaeration	13	.04	.31 (3)	.40 (1)	4	45	77
Incr Temp	1	-.01	-.15	-.17 (3)	1	1	1
HW Temp	1	-.25 (2)	-.70 (1)	-.13	1	1	1
HW DO	3	.92 (1)	.55 (2)	.04	84	8	1
Standard Deviation of Simulated DO (mg/L)					0.18	0.27	0.30
(%)					3	6	6

*( ) = rank with 1 being highest

proceeds downstream. At the downstream location, the sensivity of CBOD to point load and incremental flow inputs is strong. The sensitivity to the biochemical reaction coefficient grows in magnitude in the direction of flow, but is substantially smaller than the values associated with the point load forcing functions.

Table C-2a also presents the components of variance for the modeled CBOD output. These results show a similar, but somewhat modified pattern as the sensitivity coefficients. The headwater CBOD is the dominant contributor (99%) to CBOD variability in the upper reaches of the basin. The point load CBOD values are the primary variance component elsewhere in the river (84% at RM 20 and 79% at RM 2). The variance contribution from the CBOD rate coefficient grows in importance as one proceeds downstream, but is at least an order of magnitude lower than that from the CBOD point loads. In the downstream portion of the basin, the variance contributions from the headwater inputs are small, as one would expect. It is interesting to note that although the hydraulic inputs (incremental, point load, and headwater flow) have sensitivity coefficients that rank high, their contribution to CBOD variance is low because the relative standard deviation of these inputs is low (3%) compared to the CBOD loads (15%). The sensitivity coefficients and components of variance results at the sag point (RM 20) clearly show the upstream to downstream transition of the dominant input components. The total variability in simulated CBOD estimated by the first order analysis, when expressed as a standard deviation, varies from 0.35 mg/L to 0.76 mg/L to 0.27 mg/L as one proceeds through the basin. This prediction error is approximately 15% and is comparable to the magnitude of the error in the CBOD input forcing functions.

The FOEA results for dissolved oxygen are presented in Table C-2b. As contrasted with CBOD, the only forcing functions having large DO sensitivity coefficients are the headwater inputs, not the point load inputs. Furthermore, DO is much more sensitive to temperature inputs than is CBOD. As with CBOD, practically all the DO sensitivity in the upper reaches can be attributed to headwater DO; however as one proceeds downstream, DO loses sensitivity to the headwater condition. Next in importance in terms of DO sensitivity are the reaeration rate coefficient and velocity, both characteristic of system hydraulics. The biochemical factors of sediment oxygen demand and CBOD rate coefficient follow in rank.

Similar patterns of dissolved oxygen sensitivity are apparent from examining the components of variance (Table C-2b). The importance of reaeration and SOD is striking as is the relatively small impact of CBOD decay. The temperature inputs, while having large sensitivity coefficients, provide a minimum contribution to DO variance. Although algae dynamics were simulated in this application, their effect on DO uncertainty was negligible both in terms of sensitivity coefficient and components of variance. The total variability in simulated DO when expressed as a standard deviation increases in the downstream direction varying from 0.18 mg/L to 0.30 mg/L and averaging about 5% of the simulated DO.

D. Effect of Model Non-linearity

First order error analysis uses the linear approximation to compute an estimate of output variance. The validity of that approximation can be assessed by computing the sensitivity coefficients for both large and small values of ΔX, the input perturbation (see Eq. VI-2). Small changes in the normalized sensitivity coefficient indicate near linearity of the state variable over the range of perturbed input values, whereas large changes in sensitivity reflect important nonlinear effects. Table C-3 contains values of the normalized sensitivity coefficients for the state variables DO and chlorophyll a for input pertubations, ΔX, ranging from -20 to +20 percent. The input variables selected for analysis are those having the largest sensitivity coefficients.

For dissolved oxygen (Table C-3a), the reaeration and headwater temperature inputs show the largest relative changes in sensitivity, indicating that these variables have the largest nonlinear effects on DO. The relative changes in sensitivity coefficient for the two inputs, however, are only 9 and 16%, respectively, suggesting that the nonlinear effects are not

TABLE C-3 Normalized Sensitivity Coefficients for Various Sizes of Input Perturbations (Withlacoochee RM 20)

(a) Simulation Variable: Dissolved Oxygen (ug/L)

Input Variable	Magnitude of Input Perturbation % -20%	-1%	+1%	+20%	Relative Change (%)
CBOD Decay	-.12	-.12	-.12	-.12	0
SOD	-.23	-.23	-.22	-.23	0
Reaeration	.33	.31	.31	.30	-9
HW Temp	-.66	-.69	-.70	-.77	+16
HW DO	.55	.55	.55	.55	0
Std. Dev. (mg/L)	.28	.27	.27	.26	-7

(b) Simulation Variable: (Chlorophyll a (ug/L)

Input Variable	-20%	-1%	+1%	+20%	Relative Change (%)
Max Growth Rate	.40	.41	.42	.43	+7
Respiration	-.37	-.36	-.35	-.34	-8
Chl a/Agy-B	-1.24	-1.01	-.98	-.83	-33
HW Flow	.28	.24	.25	.21	-25
HW Chl a	.96	.95	.96	.94	-2
Std. Dev. (ug/L)	3.72	3.12	3.06	2.64	-29

strong. The other three variables, CBOD decay, SOD, and headwater DO have normalized sensitivity coefficients that are essentially constant. Thus their impacts are, for practical purposes, linear for the conditions of this simulation. The net effect from all model input nonlinearities is manifest in the FOEA estimate of dissolved oxygen standard deviation, which decreases by 7% as the magnitude of the input perturbation changes fom -20 to +20 percent.

Similar, but more pronounced patterns are observed for the state variable, chlorophyll a (Table C-3b). Two input variables, the ratio of chlorophyll a to algal biomass (Chla/Agy-B) and headwater flow exhibit large nonlinear effects on chlorophyll a. The maximum algal growth rate and the algal respiration rate show modest nonlinearities in sensitivity, while sensitivity to headwater chlorophyll a is essentially constant. The net FOEA estimate of standard deviation of chlorophyll a decreases by 29% over the range of input perturbations. Thus the effects of model nonlinearities appear to be stronger with chlorophyll a than with dissolved oxygen.

Analysis of other state variables showed changes in FOEA estimates of standard deviation of about 7% for algal growth rate, 5% for temperature and less than 5% for all others, including CBOD, the nitrogen forms and the phosphorus forms (see Table C-5). Note that, in all cases, the FOEA estimate of standard deviation decreases as the magnitude of the input perturbation increases over the range of -20 to +20%. It is curious that the large effect of model nonlinearities to chlorophyll a are not reflected in the dissolved oxygen sensitivites. This observation is perhaps explained by the fact that the largest input contributor to nonlinearity effects on chlorophyll a is a units conversion factor--the ratio of chlorophyll a to algal biomass. This factor does not serve as a linkage between the chlorophyll a and dissolved oxygen kinetic expressions in QUAL2E. The algal growth and respiration rates do provide that linkage, however, and the extent of their nonlinearities are comparable with that of dissolved oxygen, about 7%.

E. Monte Carlo Simulations

The monte carlo simulation output in QUAL2E-UNCAS provides summary statistics and frequency distributions for the state variables at specific locations in the basin. Table C-4 contains the mean, minimum, maximuim, range, standard deviation, coefficient of variation, and skew coefficient for simulated dissolved oxygen and chlorophyll a at the upstream, midpoint, and downstream locations in the Withlacoochee basin. All summary statistics are based on 2000 monte carlo simulations using the same input variances that were employed in the first order error analysis. Input probability distributions were assumed to be normal.

There is very good agreement between the calibrated mean and simulated mean for dissolved oxygen. Differences are less than 0.5%. The differences between calibrated and simulated means for chlorophyll a average about 3% and may be attributed in part to the previously described nonlinearities in chlorophyll a. For dissolved oxygen, the standard deviation grows in the

TABLE C-4 Summary Statistics from 2000 Monte Carlo Simulations for Withlacoochee River

Statistic	Dissolved Oxygen (mg/L) RM 26	RM 20	RM 2	Chlorophyll a (ug/L) RM 26	RM 20	RM 2
Calibrated Mean	5.83	4.48	5.06	18.1	14.4	6.6
Simulated Mean	5.82	4.47	5.05	18.9	15.0	6.6
Minimum	5.26	3.47	3.69	10.2	2.8	3.0
Maximum	6.41	5.31	5.89	53.8	41.4	22.2
Range	1.15	1.84	2.20	45.6	33.6	19.2
Std. Deviation	0.18	.28	.31	4.25	3.48	1.87
Coef. Variation	3.0%	6.2%	6.2%	23.5%	24.2%	28.4%
Skew Coef.	.01	-.15	-.20	1.73	1.60	1.46
Std. Deviation from FOEA	0.18	0.27	0.30	3.54	2.94	1.62

downstream direction. This phenomenon is attributable to the fact that dissolved oxygen never recovers to approach saturation (it lies in the 50 to 70% range) and to the cumulative effect of model input uncertainty as it propagates through the system. For chlorophyll a, the standard deviation decreases steadily in the downstream direction principally because the algal biomass concentration is also decreasing. The decrease in algal biomass concentration results from a lower algal growth rate attributable to reduced light penetration caused by color in the industrial waste discharge at RM 24 and to the dilution effects from groundwater inflow. The coefficient of variation for chlorophyll a averages about 25% throughout the basin, whereas that for dissolved oxygen is about 5%. The dissolved oxygen data exhibit little skew, but the chlorophyll a data show marked positive skewness.

Estimates of output variance by monte carlo simulation are not affected by model nonlinearities. Thus a comparison of monte carlo generated standard deviations with those produced by first order error analysis should provide information on the extent of any nonlinearities. As shown in Table C-4, these two estimates differ by less than 5% for DO and by about 20% for chlorophyll a. This comparison indicates weak nonlinearities associated with dissolved oxygen and more substantial ones with chlorophyll a, thus supporting the previous sensitivity coefficient observations in the first order error analysis. As shown in Table C-5, for the output variables of temperature, CBOD, and algal growth rate, the monte carlo estimate of standard deviation differs by less than 5% from the FOEA estimate. These differences are within the 95% confidence interval for the monte carlo estimates, thus implying negligible nonlinear effects for the conditions of this simulation. The frequency distributions for dissolved oxygen generated by the monte carlo analysis are shown graphically in Figure C-3. These distributions are useful in providing a visual representation of the distribution of model output at different locations in the system. In the case of dissolved oxygen shown in Figure C-3, the distributions appear nearly symmetric and the dispersion in the upper reaches of the basin is substantially smaller than that in the middle and lower reaches. Similar plots (not shown) for chlorophyll *a* data in Table C-4 clearly show the decreasing dispersion and pronounced positive skew in the simulated data.

F. Number of Monte Carlo Simulations.

A number of experiments were performed with the Withlacoochee data set to determine the number of monte carlo simulations required to achieve a given precision in the computed standard deviation of each output state variable. Twenty replicate sets of 25, 50, 100, 200, and 500 monte carlo simulations were conducted. The approximte 95% confidence interval (based on the assumption of normality) was computed for each replicate set and then plotted versus the total number of simulations performed. The results for dissolved oxygen and CBOD are presented in Figure C-4. The smooth curve represents an envelope for the upper limit of the 95% CI for simulated standard deviation from repeated monte carlo simulations. For both DO and CBOD it can be seen that about 1000 simulations are required to estimate the output standard deviation to within 5% of the mean. With this criterion as a goal, 2000 monte carlo simulations were conservatively and routinely performed for the preceding analyses.

TABLE C-5 Differences in Standard Deviation Estimates for Output Variables - Withlacoochee River Survey - 1984

Output Variables	Between FOEA Input Perturbations from -20 to +20%	Between FOEA (5%) and Monte Carlo Simulations (2000)
Temperature	5.4	1.8 - 4.3
Dissolved Oxygen	7.7	0.6 - 4.5
CBOD	0.8	1.4 - 2.6
Nitrogen Forms	*	*
Phosphorus Forms	*	*
Chlorophyll *a*	29	16 - 21
Algal Growth Rate	6.9	2 - 4

*Expected values of standard deviations too small to compute meaningful relative differences, although values are certainly less than 10% and likely less than 5%.

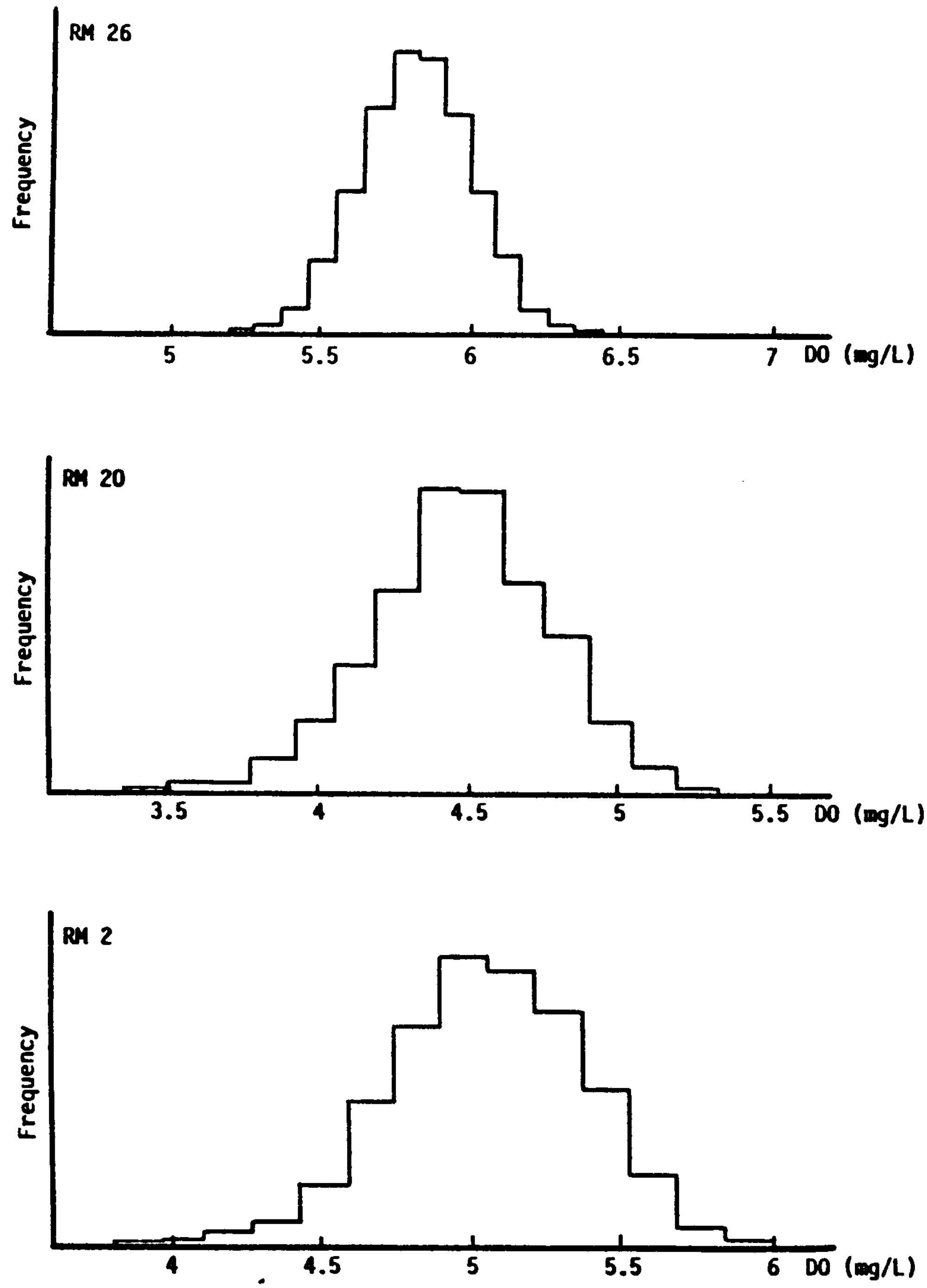

Fig. C-3. Frequency distribution for dissolved oxygen from monte carlo simulations (Withlacoochee River).

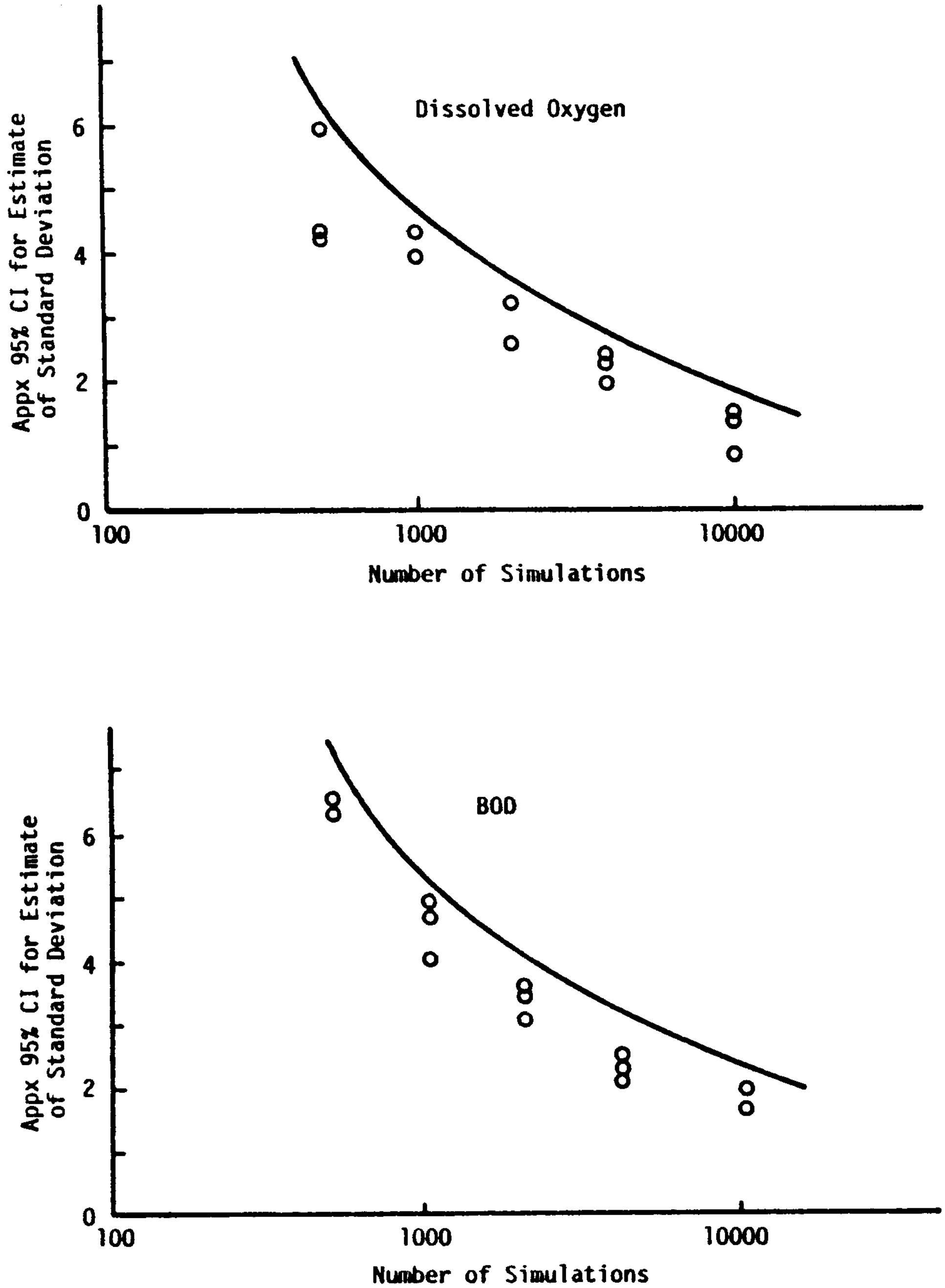

Fig. C-4. Convergence characteristics of monte carlo simulations with QUAL2E-UNCAS (Withlacoochee River).

G. Summary

The following observations summarize experience to date with uncertainty analysis using QUAL2E. QUAL2E-UNCAS has been shown to provide a useful framework for performing uncertainty analysis in steady state water quality modeling. Application of the first order error analysis and monte carlo simulation methodologies to a data set from the Withlacoochee River Basin has highlighted some of the useful features of uncertainty analysis. These include the changing sensitivities and components of variance in different portions of the river basin, the assessment of model nonlinearities, and the convergence characteristics of monte carlo methods. Better understanding of input variance and probability density functions, model nonlinearities and input parameter correlations are needed for more confident application of these techniques. An evaluation of the input factors which contribute the most to the level of uncertainty in an output variable will lead modelers in the direction of most efficient data gathering or research. In this manner the modeler can assess the risk of imprecise forecasts and recommend measures for reducing the magnitude of that imprecision.

H. Acknowledgements

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